

# On the nuclear $(n; t)$ –reaction in the three-electron ${}^6\text{Li}$ atom

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## Abstract

The nuclear  $(n; t)$ –reaction of the three-electron  ${}^6\text{Li}$  atom with thermal/slow neutrons is considered. An effective method has been developed for determining the probabilities of formation of various atoms and ions in different bound states. We discuss a number of fundamental questions directly related to numerical computations of the final state atomic probabilities. A few appropriate variational expansions for atomic wave functions of the incident lithium atom and final helium atom and/or tritium negatively charged ion are discussed. It appears that the final  ${}^4\text{He}$  atom arising during the nuclear  $(n, {}^6\text{Li}; {}^4\text{He}, t)$ -reaction in the three-electron Li atom can also be created in its triplet states. The formation of the quasi-stable three-electron  $e_3^-$  during the nuclear  $(n; t)$ –reaction at the Li atom is briefly discussed. Bremsstrahlung emitted by atomic electrons accelerated by the rapidly moving nuclear fragments from this reaction is analyzed. The frequency spectrum of the emitted radiation is investigated.

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## I. INTRODUCTION

The nuclear reaction of the  ${}^6\text{Li}$  nuclei with the thermal (and slow) neutrons is written in the form [1]

$${}^6\text{Li} + n = {}^4\text{He} + {}^3\text{H} + 4.785 \text{ MeV} \quad (1)$$

where the notations  ${}^4\text{He}$  and  ${}^3\text{H}$  stand for the helium nucleus (also the called the  $\alpha$ -particle, or  $\alpha$ , for short) and tritium (or  $t$ ) nucleus. The cross-section  $\sigma$  of this nuclear reaction for thermal neutrons with  $E_n \approx 0$  is very large  $\sigma_{max} \approx 960 \cdot 10^{-24} \text{ cm}^2$  (or 960 *barn*) [2]. The velocities of the two nuclear fragments formed in the reaction, Eq.(1), with thermal neutrons are  $v_t \approx 6.03986 \text{ a.u.}$  and  $v_\alpha \approx 4.52989 \text{ a.u.}$  for the tritium nucleus and  $\alpha$ -particle, respectively. In this study all particle velocities are given in atomic units, where  $\hbar = 1, m_e = 1, e = 1$  and the unit of atomic velocity is  $v_e = \alpha c \approx \frac{c}{137} \approx 2.1882661 \cdot 10^8 \text{ cm} \cdot \text{sec}^{-1}$ . Here and everywhere below  $c$  is the speed of light and  $\alpha = \frac{e^2}{\hbar c}$  is the dimensionless fine structure constant. This ‘atomic velocity’  $v_e$  is the velocity of the  $1s$ -electron in the hydrogen atom with the infinitely heavy nucleus  ${}^\infty\text{H}$ . It is clear that in atomic units  $v_e = 1$ .

In reality, at normal conditions the nuclear reaction, Eq.(1), occurs in the three-electron  ${}^6\text{Li}$  atom. Therefore, the electron density of the original Li atom is re-distributed somehow between the two new nuclei created in the reaction, Eq.(1). The newly created atomic nuclei move rapidly with velocities which significantly exceed average velocities of atomic electrons in the incident Li atom. The re-distribution of electron density of the incident atom between two rapidly moving nuclei leads to the three following processes: (1) formation of the final atoms and/or ions in a variety of different excited states, (2) emission of breaking radiation (or bremsstrahlung) by the accelerated electrons, and (3) formation of the spatially isolated quasi-stable three-electron system  $e_3^-$ . The first goal of this study is to evaluate the final state (atomic) probabilities for the reaction Eq.(1). Briefly, we want to determine approximate probabilities to detect the helium and tritium atoms, and  $\text{He}^+$  and  ${}^3\text{H}^-$  ions in their bound states. Note that all newly created atomic fragments from the reaction, Eq.(1), move rapidly even in the case of thermal and slow neutrons. The accurate theoretical prediction of the final state probabilities for rapidly moving atomic fragments is not trivial. Moreover, addressing this problem reveals a large number of unanswered fundamental questions. In this study we have discovered, among other things, that the final  ${}^4\text{He}$  atom can be formed not only in the singlet spin states, but in a number of triplet states also. Another interesting possibility is the

formation of the quasi-stable three-electron system  $e_3^-$  during the nuclear reaction, Eq.(1). Such system  $e_3^-$  contains no positive (heavy) particles and has a number of unique properties. In this study we also want to analyze bremsstrahlung emitted after the nuclear reaction, Eq.(1), in the three-electron Li atom. It is shown below that the frequency spectrum of such radiation essentially coincides with the well known bremsstrahlung spectrum.

## II. SUDDEN APPROXIMATION

As we have mentioned above the rate of the nuclear reaction, Eq.(1), is much faster than the rates of atomic transitions in the incident Li atom. Moreover, the two new nuclei ( $^4\text{He}$  and  $^3\text{H}$ ) arising in this reaction move with the velocities which are significantly larger than the corresponding electron velocities in the incident Li atom. This means that to determine the final state probabilities (i.e. probabilities to find newly formed atomic systems in some final states) we can apply the so-called sudden approximation [3], [4], [5]. Note also that after the nuclear reaction, Eq.(1), in the three-electron Li atom we have to deal with three new sub-systems. Two of these systems are the positively charged  $^4\text{He}$  and  $^3\text{H}$  nuclei rapidly moving from the reaction area (fast sub-systems). The third (slow) sub-system includes three electrons remaining in the reaction area, i.e. the three-electron  $e_3^-$  (or tri-electron). These three electrons are left from the incident Li atom and their wave functions still keep information about the original atom which disappeared during the nuclear reaction, Eq.(1). Interactions between these three sub-systems produce all phenomena mentioned above, i.e. formation of the different atomic species in a variety of bound (and unbound) states and emission of breaking radiation.

Suppose we want to determine the probability that the rapidly moving  $^4\text{He}$  nucleus takes one of the three atomic (Li) electrons remaining unbound after the nuclear reaction, Eq.(1). In other words, the final atomic system is the positively charged helium ion  $^4\text{He}^+$ . For an atomic system containing fast and slow sub-systems the corresponding probability is written in the form (see, e.g., [5])

$$P_{if} = \left| \int \rho_{\text{Li}}^{(1)}(\mathbf{r}_{14}) \exp(i\mathbf{V}_\alpha \cdot \mathbf{r}_{14}) \rho_{\text{He}^+}(\mathbf{r}_{14}) d^3\mathbf{r}_{14} \right| \quad (2)$$

where  $\mathbf{V}_\alpha$  is the velocity of the  $\text{He}^+$  ion after the reaction, Eq.(1) and  $\rho_{\text{Li}}^{(1)}(\mathbf{r}_{14})$  and  $\rho_{\text{He}^+}(\mathbf{r}_{14})$  are the one-electron density matrixes of the Li atom and  $\text{He}^+$  ion, respectively. These density

matrices are simply related with the corresponding wave functions of the bound states, e.g., for the one-electron density matrix of the Li atom

$$\rho_{\text{Li}}^{(1)}(\mathbf{r}_{14}) = 3 \int \int \int \Psi_{\text{Li}}^*(\mathbf{x}_{14}, \mathbf{x}_{24}, \mathbf{x}_{34}) \Psi_{\text{Li}}(\mathbf{x}_{14}, \mathbf{x}_{24}, \mathbf{x}_{34}) ds_1 d\mathbf{x}_{24} d\mathbf{x}_{34} \quad (3)$$

where  $\mathbf{x}_i = (s_i, \mathbf{r}_i)$  is the complete set of spin-spatial coordinates of the  $i$ -th electron. In Eqs.(2) - (3) and everywhere below the nucleus in the three-electron Li atom is designated by the index 4, while three electrons are denoted by the indexes 1, 2 and 3. This definition of the one-electron density matrix, Eq.(3)), and notations used in this equation correspond to the definition given in Eqs.(4.1.5) - (4.1.6) of [6]. The one-electron density matrix for the one-electron  $\text{He}^+$  ion is

$$\rho_{\text{He}^+}(\mathbf{r}_{14}) = \rho_{\text{He}^+}^{(1)}(\mathbf{r}_{14}) = \int \Phi_{\text{He}^+}^*(\mathbf{x}_{14}) \Phi_{\text{He}^+}(\mathbf{x}_{14}) ds_1 \quad (4)$$

It contains only one integral over spin variables of the electron 1.

If the tritium atom is formed during the nuclear reaction, Eq.(1) in the three-electron Li atom, then we can write the following formula for the final state probability  $P_{if}$

$$P_{if} = \int \rho_{\text{Li}}^{(1)}(\mathbf{r}_{14}) \exp(i\mathbf{V}_t \cdot \mathbf{r}_{14}) \rho_{\text{T}}(\mathbf{r}_{14}) d^3\mathbf{r}_{14} \quad (5)$$

where  $\rho_{\text{T}}(\mathbf{r}_{14})$  is the one-electron density matrix of the tritium atom. and  $\mathbf{V}_t$  is the velocity of the tritium nucleus after the nuclear reaction, Eq.(1). Here the notations T and  $t$  stand for the tritium and tritium nucleus, respectively, while  $\mathbf{V}_t$  is the velocity of the tritium nucleus after the nuclear reaction, Eq.(1).

For the helium atom product (two bound electrons) the final state probability  $P_{if}$  is written in the form

$$P_{if} = \int \int \rho_{\text{Li}}^{(2)}(\mathbf{r}_{14}, \mathbf{r}_{24}) \exp(i\mathbf{V}_\alpha \cdot \mathbf{r}_{14} + i\mathbf{V}_\alpha \cdot \mathbf{r}_{24}) \rho_{\text{He}}^{(2)}(\mathbf{r}_{14}, \mathbf{r}_{24}) d^3\mathbf{r}_{14} d^3\mathbf{r}_{24} \quad (6)$$

where  $\mathbf{V}_\alpha$  is the final velocity of the  $\alpha$ -particle after the nuclear reaction, Eq.(1). The two-electron density matrix of the three-electron Li atom is defined as follows

$$\rho_{\text{Li}}^{(2)}(\mathbf{r}_{14}, \mathbf{r}_{24}) = 6 \int \int \int \Psi_{\text{Li}}^*(\mathbf{x}_{14}, \mathbf{x}_{24}, \mathbf{x}_{34}) \Psi_{\text{Li}}(\mathbf{x}_{14}, \mathbf{x}_{24}, \mathbf{x}_{34}) ds_1 ds_2 d\mathbf{x}_{34} \quad (7)$$

where we have used the factor  $N(N-1)$  in the front of the density matrices [6]. In some cases, however, it is better to use a different definition of the density matrices with the unity factor. The two-electron density matrix of the He atom (bound states) takes the form

$$\rho_{\text{He}}(\mathbf{r}_{14}, \mathbf{r}_{24}) = \rho_{\text{He}}^{(2)}(\mathbf{r}_{14}, \mathbf{r}_{24}) = \int \Phi_{\text{He}}^*(\mathbf{x}_{14}, \mathbf{r}_{24}) \Phi_{\text{He}}(\mathbf{x}_{14}, \mathbf{r}_{24}) ds_1 ds_2 \quad (8)$$

In the case of nuclear reaction, Eq.(1), in the three electron Li atom we need only one- and two-electron density matrices, since the negatively charged  $\text{He}^-$  is unstable. Note that all these integrals mentioned in the expressions for the probabilities, Eq.(2), Eqs.(5) - (6) and density matrices, Eqs.(3) - (4) and (8), include the wave functions of the bound few-electron atoms and ions. These wave functions must be determined from accurate atomic computations, whose construction is discussed in the next Section.

### III. VARIATIONAL WAVE FUNCTION OF THE LITHIUM ATOM

To determine the final state probabilities we need to construct the accurate variational wave functions for the incident and final atomic systems involved in the reaction, Eq.(1). In our earlier paper [8] we have calculated the final state probabilities to form one-electron atoms and ions in those cases when exothermic nuclear  $(n; t)-$  and  $(n; \alpha)-$ reactions occur in one-electron atoms/ions, i.e., both incident and final atomic systems contain only one bound electron. In this study we deal with the actual three-electron wave function of the incident  ${}^6\text{Li}$  atom and two-electron wave function of the final  ${}^4\text{He}$  atom. Also, we consider the formation of the one-electron  $\text{He}^+$  ion, tritium atom  ${}^3\text{H}$  (or T) and two-electron negatively charged tritium ion  ${}^3\text{H}^-$  (or  $\text{T}^-$ ).

First, let us discuss the construction of three-electron variational wave function for the Li atom. Without loss of generality, below we restrict ourselves to the consideration of the ground  ${}^2S(L=0)-$ state of the Li atom. As is well known (see, e.g., [9], [10]) the accurate variational wave function of the ground (doublet)  ${}^2S(L=0)-$ state of the Li atom is written in the following general form

$$\Psi(\text{Li})_{L=0} = \psi_{L=0}(A; \{r_{ij}\})(\alpha\beta\alpha - \beta\alpha\alpha) + \phi_{L=0}(B; \{r_{ij}\})(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) \quad (9)$$

where  $\psi_{L=0}(A; \{r_{ij}\})$  and  $\phi_{L=0}(B; \{r_{ij}\})$  are the two independent radial parts (= spatial parts) of the total wave function. Everywhere below in this study, we shall assume that all mentioned wave functions have unit norms. The notations  $\alpha$  and  $\beta$  in Eq.(9) stand for the one-electron spin-up and spin-down functions, respectively (see, e.g., [11]). The notations  $A$  and  $B$  in Eq.(9) mean that the two sets of non-linear parameters associated with the radial functions  $\psi$  and  $\phi$  can be optimized independently. Note that each of the radial basis functions in Eq.(9) explicitly depends upon all six interparticle (or relative) coordinates

$r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}$ , where the indexes 1, 2, 3 stand for the three electrons, while index 4 means the nucleus.

The actual atomic wave function in an atomic system must be completely antisymmetric with respect to all electron spin-spatial variables. For a three-electron wave function this requirement is written in the form  $\hat{\mathcal{A}}_{123}\Psi(1, 2, 3) = -\Psi(1, 2, 3)$ , where the wave function  $\Psi$  is given by Eq.(9) and  $\hat{\mathcal{A}}_e$  is the three-particle (or three-electron) antisymmetrizer  $\hat{\mathcal{A}}_e = \hat{e} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} + \hat{P}_{132}$ . Here  $\hat{e}$  is the identity permutation, while  $\hat{P}_{ij}$  is the permutation of the  $i$ -th and  $j$ -th particles. Analogously, the operator  $\hat{P}_{ijk}$  is the permutation of the  $i$ -th,  $j$ -th and  $k$ -th particles.

Suppose that the three-electron wave function of the Li atom has been constructed in the form of Eq.(9). By applying the antisymmetrizer  $\hat{\mathcal{A}}_{123}$  to the first part of the total wave function, Eq.(9), one finds

$$\begin{aligned} \hat{\mathcal{A}}_{123}[\psi_{L=0}(A; \{r_{ij}\})(\alpha\beta\alpha - \beta\alpha\alpha)] &= (\hat{e}\psi)(\alpha\beta\alpha - \beta\alpha\alpha) + (\hat{P}_{12}\psi)(\alpha\beta\alpha - \beta\alpha\alpha) \\ &\quad - (\hat{P}_{13}\psi)(\alpha\beta\alpha - \alpha\alpha\beta) - (\hat{P}_{23}\psi)(\alpha\alpha\beta - \beta\alpha\alpha) + (\hat{P}_{123}\psi)(\alpha\alpha\beta - \alpha\beta\alpha) \\ &\quad + (\hat{P}_{132}\psi)(\beta\alpha\alpha - \alpha\alpha\beta) \end{aligned} \quad (10)$$

where the notations  $(\hat{P}_{ij}\psi)$  and  $(\hat{P}_{ijk}\psi)$  mean the permutation operators which act on the coordinate wave functions only. Analogously, for the second part of the total wave function one finds

$$\begin{aligned} \hat{\mathcal{A}}_{123}[\phi_{L=0}(B; \{r_{ij}\})(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha)] &= (\hat{e}\phi)(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) \\ &\quad - (\hat{P}_{12}\phi)(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) - (\hat{P}_{13}\phi)(2\beta\alpha\alpha - \alpha\alpha\beta - \alpha\beta\alpha) \\ &\quad - (\hat{P}_{23}\phi)(2\alpha\beta\alpha - \alpha\alpha\beta - \beta\alpha\alpha) + (\hat{P}_{123}\phi)(2\beta\alpha\alpha - \alpha\beta\alpha - \alpha\alpha\beta) \\ &\quad + (\hat{P}_{132}\phi)(2\alpha\beta\alpha - \alpha\alpha\beta - \beta\alpha\alpha) \end{aligned} \quad (11)$$

where the notations  $(\hat{P}_{ij}\phi)$  and  $(\hat{P}_{ijk}\phi)$  mean the permutations of the spatial coordinates in the  $\phi_{L=0}(B; \{r_{ij}\})$  radial function, Eq.(9).

Now, by using the formulas, Eqs.(10) and (11), we can obtain the formulas which can be used in computations of the final state probabilities in the case of nuclear reaction, Eq.(1), in the three-electron Li atom. For instance, if the final wave function has the same spin-symmetry, i.e. it is written in the form

$$\Psi_{fi} = \psi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)(\alpha\beta\alpha - \beta\alpha\alpha) + \phi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) \quad (12)$$

then the final state probabilities are determined with the use of the following formulas

$$P_{\psi\psi} = \langle \psi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2\sqrt{3}} (2\hat{e} + 2\hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132}) \psi_{Li}(A; \{r_{ij}\}) \rangle \quad (13)$$

$$P_{\phi\psi} = \langle \phi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2} (\hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} - \hat{P}_{132}) \psi_{Li}(A; \{r_{ij}\}) \rangle \quad (14)$$

$$P_{\psi\phi} = \langle \psi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2} (\hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} - \hat{P}_{132}) \phi_{Li}(B; \{r_{ij}\}) \rangle \quad (15)$$

$$P_{\phi\phi} = \langle \phi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2\sqrt{3}} (2\hat{e} - 2\hat{P}_{12} + \hat{P}_{13} + \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132}) \phi_{Li}(B; \{r_{ij}\}) \rangle \quad (16)$$

Note that these formulas coincide with the known formulas [12] which correspond to the doublet  $\rightarrow$  doublet transition in the three-electron atomic systems. Briefly, this means that the both incident and final atomic states contain three-electrons in the doublet spin configuration (the total electron spin equals  $\frac{1}{2}$ ).

By considering all possible spin configurations for the final atomic state one finds that other spin configurations are possible. For instance, if reaction Eq.(1) leads to the formation of the two neutral atoms ( $^4\text{He}$  and  $^3\text{H}$  atoms), then the helium atom can be detected either in the singlet state, or in the triplet state. The spin function of the singlet state is  $\chi_s = \frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$ , while the wave function of the triplet state can be chosen (in our case) in the form  $\chi_t = \alpha\alpha$ . It is clear that these two wave functions have unit norms and they are orthogonal to each other. The probability of formation of the  $^4\text{He}$  atom in its singlet spin state is determined by the formulas, Eqs.(13) - (16). The tritium atom in this case will be formed with the  $\beta$ -electron spin function.

If the final state of the  $^4\text{He}$  atom is the triplet state ( $tr$ ), then the formulas for the final state probabilities take the form

$$P_{tr;\psi} = \langle \psi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2} (\hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} - \hat{P}_{132}) \psi_{Li}(A; \{r_{ij}\}) \rangle \quad (17)$$

$$P_{tr;\phi} = \langle \psi_{fi}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \frac{1}{2\sqrt{3}} (2\hat{e} - 2\hat{P}_{12} + \hat{P}_{13} + \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132}) \phi_{Li}(B; \{r_{ij}\}) \rangle \quad (18)$$

These formulas indicate clearly that the probability to find the  $^4\text{He}$  atom arising during the nuclear reaction, Eq.(1), in its triplet spin state(s) is not zero. In all earlier studies the transitions to the final atomic states with different spin states was ignored (never considered).

#### IV. FORMATION OF THE TRI-ELECTRON

As mentioned above the two nuclear fragments formed in the reaction, Eq.(1), move with very large velocities. They leave the reaction zone very quickly for a time which

is significantly shorter than a typical atomic time  $\tau_a = \frac{\hbar^3}{m_e e^4} \approx 2.42 \cdot 10^{-17} \text{ sec}$ . The three negatively charged electrons  $e^-$  remain in the reaction zone substantially longer. The arising quasi-stable system of three electrons  $e_3^-$  is called a three-electron, or tri-electron. It is clear that the tri-electron is not a stable system and after some time it will be destroyed by the Coulomb repulsion between electrons. However, in some cases such a destruction takes a relatively long time which is sufficient to detect it experimentally and measure some of its properties. A combination of the stabilizing electric and magnetic fields can be used to increase the life-time of a tri-electron. Some of the properties of the  $e_3^-$  system can be studied by using modern methods of the femto- and attosecond physics. Experimental interest to study such new systems cannot be overestimated.

The ‘quasi-atomic’ tri-electron system has a large number of unique properties and can be considered as a light quasi-atom which has no central (i.e. heavy), positively charged nucleus. In the case of reaction, Eq.(1), the spin-spatial symmetry of the three-electron wave function exactly coincides with the corresponding symmetry of the wave function of the ground  $^2S$ -state of the Li atom.

## V. CALCULATIONS

In this study we have developed an approximate procedure to construct the bound state wave functions of the three-electron atoms and ions. This procedure can be used to perform numerical evaluations of the final state probabilities in the case of the nuclear reaction, Eq.(1), and for the  $\beta^-$ -decaying isotopes of the three-electron atoms [13]. In this approach the trial wave function is constructed as the sum of various terms and each of these terms contains the products of the electron-nucleus functions. None of the three electron-electron coordinates  $r_{32}, r_{31}, r_{21}$  is included in such trial wave functions. This simplifies drastically the following Fourier transforms of such wave functions. For the ground state (the doublet  $^2S(L=0)$ -state) of the Li atom the radial wave function  $\psi_{L=0}(A; \{r_{ij}\})$  is chosen in the following form:

$$\begin{aligned} \psi_{L=0}(r_{14}, r_{24}, r_{34}, 0, 0, 0) &= \sum_{k=1}^{N_s} C_k r_{14}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} \exp(-\alpha_k r_{14} - \beta_k r_{24} - \gamma_k r_{34}) \\ &= \sum_{k=1}^{N_s} C_k r_1^{m_1(k)} r_2^{m_2(k)} r_3^{m_3(k)} \exp(-\alpha_k r_1 - \beta_k r_2 - \gamma_k r_3) \end{aligned} \quad (19)$$



where  $C_k$  are the linear (or variational) coefficients, while  $m_1(k), m_2(k)$  and  $m_3(k)$  are the three integer (non-negative) parameters, which are, in fact, the powers of the three electron-nucleus coordinates  $r_{i4} = r_i$  ( $i = 1, 2, 3$ ). The real (and non-negative) parameters  $\alpha_k, \beta_k, \gamma_k$  are the  $3N_s$  varied parameters of the variational expansion, Eq.(19). Below, we shall assume that the trial wave function Eq.(19) has a unit norm. Furthermore, in all calculations performed for this study only one spin function  $\chi_1$  ( $\chi_1 = \alpha\beta\alpha - \beta\alpha\alpha$ ) is used. The wave function, Eq.(19), must be properly anti-symmetrized upon all spin-spatial coordinates of the three electrons.

The principal question for the wave function, Eq.(19), is related to its overall accuracy. If (and only if) such accuracy is relatively high, then such a wave function, Eq.(19), can be used in actual computations of the probability amplitudes. In this study we have constructed the 23-term variational wave function shown in Table I. This wave function is represented in the form of Eq.(19) and contains no electron-electron coordinates. All sixty nine ( $69 = 3 \times 23$ ) non-linear parameters  $\alpha_k, \beta_k, \gamma_k$  ( $k = 1, 2 \dots 23$ ) in this wave function have been optimized carefully in a series of bound state computations performed for the ground state of the Li atom. Finally, the total energy  $E$  of the ground  $^2S$ -state of the  $^\infty\text{Li}$  atom obtained with this 23-term trial wave function, Eq.(19), was  $-7.44859276608 \text{ a.u.}$  This energy is close to the exact total energy of the ground state of the  $^\infty\text{Li}$  atom. It indicates a good overall quality of our approximate wave function with 23 terms which does not include any of the electron-electron coordinates  $r_{12}, r_{13}, r_{23}$ . This wave function is used in the computations of the final state probabilities (see below) for the nuclear reaction, Eq.(1), in three-electron Li atom.

Note also that in atomic physics based on the Hartree-Fock and hydrogenic approximations the ground state in the Li atom is designated as the  $2^2S$ -state, while in the classification scheme developed in highly accurate computations the same state is designated as the  $1^2S$ -state because it corresponds to the first eigenvalue of the Hamiltonian matrix  $\hat{H}$ . This classification scheme is very convenient for truely correlated few-electron wave functions which represent situation where there are no good hydrogenic quantum numbers. Nevertheless, to avoid conflicts between these two classification schemes in this study we follow the system of notation used earlier by Larsson [9] which designated this state of the Li atom as the ‘ground  $^2S$ -state’.

The advantage of the basis functions, Eq.(19), for numerical calculations of the final state

probabilities for the reaction Eq.(1) is two-fold: (1) these trial wave functions allow one to obtain relatively accurate approximations for atomic three-electron wave functions; and (2) all required Fourier transforms are easily performed for such trial wave functions since they do not include electron-electron coordinates. Note also, that approximate two-electron wave functions of the He atom and/or  $H^-$  ion can be constructed in analogous form which contain only electron-nucleus coordinates, e.g.,

$$\psi_{L=0}(r_1, r_2, 0) = \frac{1}{\sqrt{2}}(1 + \hat{P}_{12}) \sum_{k=1}^{N_s} C_k r_1^{m_1(k)} r_2^{m_2(k)} \exp(-\alpha_k r_1 - \beta_k r_2) \quad (20)$$

Some probabilities (in %) of observing selected electron final states in the helium ion  $^4\text{He}^+$  and tritium atom  $^3\text{H}$  arising in the exothermic nuclear reaction Eq.(1) of the three-electron lithium-6 atom can be found in Table II. In calculations included in Table II we have assumed that the incident Li atom was in its ground  $^2S$ -state. Also, we assume that the nuclear  $(n; t)$ -reaction, Eq.(1), proceeds is produced by thermal and/or slow neutrons.

## VI. BREMSSTRAHLUNG

As we have mentioned above the two positively charged atomic nuclei created in the nuclear reaction, Eq.(1), with thermal neutrons move with substantial velocities in the two opposite directions. In general, these two positively charged nuclei will produce acceleration of electrons which still remain in the reaction zone. In turn, the accelerated electrons will generate emission of radiation. It appears that the spectrum of this radiation essentially coincides with the known spectrum of bremsstrahlung (or breaking radiation). In this Section we discuss the basic properties of radiation emitted during the nuclear reaction, Eq.(1), in three-electron  $^6\text{Li}$  atom.

Note that the reaction, Eq.(1), is a fission-type reaction in a three-electron atomic system. The original nucleus decays into two electrically charged fragments which are rapidly moving away from each other. The general theory of radiation emitted during such processes was developed in our earlier studies (see, e.g., [8], [14] and references therein). Atomic electrons from outer electronic shells become free during this fission-type nuclear reaction in an atomic nucleus. These free electrons interact with the rapidly moving nuclear fragments and such an interaction can produce breaking radiation or bremsstrahlung. Here we want to derive the explicit formulas for this radiation and investigate its spectrum. The electric charges

and velocities of these fission fragments are  $Q_1e, Q_2e$  and  $V_1, V_2$ , respectively. To simplify all formulas below, we shall assume that the both fission fragments move along the  $Z$ -axis. Furthermore, in this study we restrict ourselves to the consideration of the non-relativistic processes only (i.e. the two velocities  $V_1, V_2$  are significantly less than the speed of light  $c$  in vacuum). The case of arbitrary velocities is discussed in [14].

The electron acceleration is directly related to the second time-derivative of the dipole moment, i.e.  $\ddot{\mathbf{d}} = e\ddot{\mathbf{r}}$ , where  $\mathbf{d}$  is the dipole moment. In the case of fission-type reaction in atomic systems the explicit formula for electron's acceleration is

$$\ddot{\mathbf{r}} = \frac{1}{m_e} \left[ \nabla \left( \frac{Q_1 e^2}{R_1} \right) + \nabla \left( \frac{Q_2 e^2}{R_2} \right) \right] = \frac{Q_1 e^2}{m_e} \nabla \left( \frac{1}{R_1} \right) + \frac{Q_2 e^2}{m_e} \nabla \left( \frac{1}{R_2} \right) \quad (21)$$

where  $R_1 = \sqrt{x^2 + y^2 + (z - V_1 t)^2}$  and  $R_2 = \sqrt{x^2 + y^2 + (z + V_2 t)^2}$ . The notations  $V_1$  and  $V_2$  stand for the velocities of the two fission fragments. The second time-derivative of the dipole moment is

$$\ddot{\mathbf{d}} = \frac{Q_1 e^3}{m_e} \nabla \left( \frac{1}{R_1} \right) + \frac{Q_2 e^3}{m_e} \nabla \left( \frac{1}{R_2} \right) = -\frac{Q_1 e^3}{m_e} \frac{\mathbf{R}_1}{R_1^3} - \frac{Q_2 e^3}{m_e} \frac{\mathbf{R}_2}{R_2^3} \quad (22)$$

where  $\mathbf{R}_1 = (x, y, z - V_1 t)$  and  $\mathbf{R}_2 = (x, y, z + V_2 t)$  are the three-dimensional vectors. The intensity of the non-relativistic bremsstrahlung from a fission-type reaction in a one-electron atomic system is

$$dI = \frac{1}{4\pi c^3} (\ddot{\mathbf{d}} \times \mathbf{n})^2 d\Omega = \left( \frac{e^2}{m_e} \right)^2 \frac{Q^2 e^2}{4\pi c^3} \left[ \frac{Q_1}{Q} \frac{\mathbf{R}_1}{R_1^3} + \frac{Q_2}{Q} \frac{\mathbf{R}_2}{R_2^3} \right]^2 \sin^2 \theta d\Omega \quad (23)$$

where  $\theta$  is the angle between the vector  $\ddot{\mathbf{d}}$  and vector  $\mathbf{n}$  which designates the direction of propagation of radiation. The notation  $Q$  in the last equation stands for an arbitrary electric charge. This value can be considered as an output parameter. In particular, one can choose  $Q = Q_1$ , or  $Q = Q_2$ . For a  $N_e$ -electron atomic system the last formula takes the form

$$dI = \left( \frac{e^2}{m_e} \right)^2 \frac{N_e Q^2 e^2}{4\pi c^3} \left[ \frac{Q_1}{Q} \frac{\mathbf{R}_1}{R_1^3} + \frac{Q_2}{Q} \frac{\mathbf{R}_2}{R_2^3} \right]^2 \sin^2 \theta d\Omega \quad (24)$$

This formula can be re-written in the form

$$\frac{dI}{d\Omega} = \left( \frac{e^2}{m_e} \right)^2 \frac{N_e Q^2 e^2}{4\pi c^3} \left[ \frac{Q_1^2}{Q^2} \frac{1}{R_1^4} + \frac{Q_2^2}{Q^2} \frac{1}{R_2^4} + \frac{Q_1 Q_2}{Q^2} \left( \frac{\mathbf{R}_1 \cdot \mathbf{R}_2}{R_1^3 R_2^3} \right) \right]^2 \sin^2 \theta \quad (25)$$

for the differential cross-section. Our derivation of these formulas is based on the fact that radiation emitted by different post-atomic electrons is non-coherent. Indeed, the three free electrons arising during the reaction, Eq.(1), are independent quantum systems and they

move as ‘random’ particles. It can be shown that the ‘randomization’ of the phases of the electron wave functions is directly related to the electron-electron repulsion which was ignored in Eqs.(21) - (23). At certain conditions bremsstrahlung from fission-type process in atomic systems can be coherent. For instance, if two fission fragments move with very large velocities, while all post-atomic electrons almost do not move at the beginning of the process. In this case, one needs to introduce an additional factor  $N_e$  in the last formula.

Let us discuss the spectrum of the emitted radiation. As follows from the formula, Eq.(25), the intensity of bremsstrahlung from fission-type processes in atomic systems rapidly decreases with the time  $I \simeq t^{-4}$  after the nuclear reaction ( $t = 0$ ). Such a behaviour is typical for all finite-time process/reactions with accelerated electrons. The spectral resolution  $R(\omega)$  (or spectral function) of the intensity of dipole radiation is written in the form

$$dR(\omega) = \frac{4}{3c^3} |\ddot{\mathbf{d}}_\omega|^2 \frac{d\omega}{2\pi} = \frac{4\omega^4}{3c^3} |\mathbf{d}_\omega|^2 \frac{d\omega}{2\pi} \quad (26)$$

where  $\mathbf{d}_\omega$  is the Fourier component of the dipole moment  $\mathbf{d}$  defined above. As follows from Eq.(26) one needs to find the Fourier components of the vector of the dipole moment  $\ddot{\mathbf{d}}_\omega$ , Eq.(21). Finally, the problem is reduced to the calculation of the two following Fourier transformations

$$I_1(\omega; \frac{a}{V}, V, \cos \eta) = \int_0^{+\infty} \left[ \frac{a^2}{V^2} \pm 2(\frac{a}{V} \cos \eta) \cdot t + t^2 \right]^{-\frac{3}{2}} \exp(i\omega t) dt \quad (27)$$

and

$$I_2(\omega; \frac{a}{V}, V, \cos \eta) = \int_0^{+\infty} \left[ \frac{a^2}{V^2} \pm 2(\frac{a}{V} \cos \eta) \cdot t + t^2 \right]^{-\frac{3}{2}} t \exp(i\omega t) dt \quad (28)$$

where  $a$  is the ‘effective’ radius of the original electron shell and  $\eta$  is the angle between the electron acceleration and  $Z$ -axis (or the line along which the two nuclei are moving). Note that the spectrum of the emitted radiation depends upon  $\cos \eta$ , as for all fission-type reactions and processes. The lower limit in these formulas is zero, but, in reality, we cannot use times  $t$  which are shorter than  $\tau = \frac{a}{c}$ . Formally, this means that the lower limits in Eqs.(27) and (28) can slightly be changed and this can be used to simplify the explicit formulas for the corresponding Fourier components. The actual upper limits in Eqs.(27) and (28) are also finite. For instance, it is possible to obtain a very good approximation for the integrals, Eqs.(27) and (28), by using the upper limit  $\frac{10a}{V}$ . In actual situations one can use the formula  $\exp(ix) = \cos x + i \sin x$  and then calculate all arising integrals numerically,

or by using analytical formulas from the Tables of Fourier *sine/cosine* transformations (see, e.g., [15]).

To produce the explicit formula for the spectral functions  $I_1(\omega; \frac{a}{V}, V, \cos \eta)$  and  $I_2(\omega; \frac{a}{V}, V, \cos \eta)$  we note the following relation between these two functions:

$$I_2(\omega; \frac{a}{V}, V, \cos \eta) = -i \frac{\partial}{\partial \omega} I_1(\omega; \frac{a}{V}, V, \cos \eta) \quad (29)$$

This formula substantially simplifies the computation of the Fourier transformations. Moreover, a very good approximation for the  $I_1(\omega; \frac{a}{V}, V, \cos \eta)$  function is:

$$I_1(\omega; \frac{a}{V}, V, \cos \eta) = \exp\left(-i\omega \frac{a}{V}, \cos \eta\right) \left[ \frac{\omega}{b} K_1(b\omega) + \frac{1}{\omega} \ln\left(\frac{1 + \frac{1}{2}b\omega}{1 - \frac{1}{2}b\omega}\right) - \frac{\pi}{4} \frac{\omega^2}{(1 - \frac{1}{2}b\omega)^2} \right] \quad (30)$$

where  $b = \frac{a \sin \eta}{V}$  and  $K_1(x)$  is the MacDonald function (see, e.g., [16]). The formula, Eq.(30), describes the spectrum of radiation emitted by one electron accelerated by rapidly moving atomic fragments from the nuclear  $(n, {}^6\text{Li}; {}^4\text{He}, t)$ -reaction. The actual spectra emitted during the nuclear  $(n, {}^6\text{Li}; {}^4\text{He}, t)$ -reaction in the three-electron Li atom can be different from the spectrum predicted by the formula Eq.(30) since we have ignored all contributions from the electron-electron repulsion(s). It is interesting to study such radiation in detail. In general, the intensity of bremsstrahlung from the reaction, Eq.(1), can be amplified by accelerating the incident  ${}^6\text{Li}$  atom or  ${}^6\text{Li}^+$  ion to very large velocities.

## VII. CONCLUSION

We have considered the nuclear reaction, Eq.(1), with the thermal/slow neutrons in the three-electron Li atom. It is shown that a number of different atoms and ions can be formed during this reaction. This also includes the formation of the electrically charged tri-electron  $e_3^-$  ion which is a quasi-stable negatively charged ion. It has the same (doublet) symmetry as the wave function of the incident Li atom. We have developed an effective method for accurate evaluation of the final state probabilities, i.e. probabilities to form different atomic species in a variety of bound states. This method is based on the use of special three- and two-electron wave functions of the Li and He atoms, respectively, whose explicit form allows one to obtain accurate numerical results for all bound state properties of the incident and final atoms/ions. On the other hand, for the same wave functions it is easy to perform all complete and/or partial Fourier transformations needed in calculations of the final state

probabilities. The spectrum of the emitted radiation has been investigated. It is shown that such a spectrum essentially coincides with the known spectrum of bremsstrahlung emitted by the accelerated electrons.

Our procedure can now be used for the more complicated nuclear  $(n; \alpha)$ -reaction in the five-electron B-atom (see Appendix). The  $(n, {}^{10}\text{B}; {}^7\text{Li}, \alpha)$ -reaction on this atom is of great interest in a number of applications, e.g., in medical physics (BNCT). The Li-atom/ion and He-atom/ion which are formed during this reaction may contain up to three and two electrons, respectively. These atomic fragments move rapidly, with the velocities  $v_{Li} \approx 2.40896 \text{ cm} \cdot \text{sec}^{-1}$  and  $v_{\alpha} \approx 4.21568 \text{ cm} \cdot \text{sec}^{-1}$  in the case of slow neutrons. The sudden approximation can certainly be applied to the He-atom and He-like ions. However, this approximation cannot be used for internal electrons (or  $1^2s$ -electrons) of the Li atom/ion, since the velocities of these two electrons are comparable with the final velocity of the  ${}^7\text{Li}$  nucleus. It is very likely that the probability to observe the  ${}^7\text{Li}^{2+}$  ions after Eq.(31) will be relatively small  $\leq 5 - 10 \%$ , while analogous probability for the  ${}^7\text{Li}^+$  ions will be relatively large ( $\geq 50 \%$ ).

## Appendix

In this study our analysis was restricted to the consideration of the nuclear  $(n; t)$ -reaction, Eq.(1), in the three-electron Li atom. Moreover, such a reaction is considered for thermal and slow neutrons only. In reality, the nuclear reaction of the  ${}^6\text{Li}$  nucleus, Eq.(1), proceeds with neutrons of all energies and the energy released increases almost linearly with the energy of the incident neutron. For fast neutrons with  $E_n \geq 1 \text{ MeV}$  the energy released is substantially different from the value quoted in Eq.(1) and the velocities of the atomic fragments increase correspondingly. Investigation of the final state (atomic) probabilities and bremsstrahlung emitted during such processes with fast neutrons is of interest in some applications. Note that the cross-section of this reaction has a large resonance (maximum)  $\sigma \approx 4.5 \text{ barn}$  at  $E_n \approx 240 - 270 \text{ keV}$ , but it is relatively large for neutrons of all energies  $E_n \leq 0.8 \text{ MeV}$ . This makes the reaction, Eq.(1), extremely important in the thermonuclear ignition and following propagation of the thermonuclear burning wave in highly compressed ( $\rho \geq 100 \text{ g} \cdot \text{cm}^{-3}$ )  ${}^6\text{LiD}$  deuteride which is routinely used as a fuel in modern thermonuclear explosive devices (see, e.g., [17], [18]). The analogous  $(n, {}^3\text{He}; p, t)$ -reaction [8] also plays a very important role in such processes.

In general, the nuclear  $(n, t)$ -reactions of the  ${}^6\text{Li}$  and  ${}^3\text{He}$  nuclei with neutrons allow one to reduce drastically the overall bremsstrahlung loss from the hot combustion zone and increase the tritium/deuterium ratio which is crucially important to start new thermonuclear  $(d, t)$ -reactions. Briefly, by using the  ${}^6\text{LiD}$  deuteride in modern thermonuclear explosive devices we can reduce the required compressions to relatively small values. In many cases such compressions are dozens times smaller (usually, in 25 - 40 times smaller [18]) than compressions required for any other (solid) thermonuclear fuel, e.g.,  ${}^7\text{LiD}$  deuteride. On the other hand, by using compressions which are provided by a standard ‘primary’ nuclear charge one can create extremely compact thermonuclear explosive devices based on  ${}^6\text{LiD}$  deuteride. The idea to use pure  ${}^6\text{LiD}$  deuteride in thermonuclear explosive devices was originally proposed by V.L. Ginzburg in 1948-1949 (see discussion and references in [17]).

Some other  $(n; t)$ -,  $(n; p)$ - and  $(n; \alpha)$ -reactions are often used in different applications. For instance, the nuclear reaction of  ${}^{10}\text{B}$  nuclei with slow neutrons

$${}^{10}\text{B} + n = {}^7\text{Li} + {}^4\text{He} + 2.791 \text{ MeV} \quad (31)$$

is extensively used in the boron neutron capture therapy (BNCT, for short), or boron neutron-capture synovectomy [19] - [23], to treat different forms of cancer, including brain cancer. The fast  $\alpha$ -particle produced in the reaction, Eq.(31), kills (or at least ‘badly damages’) one cancer cell before it finally stops. The modern applications of this reaction to cancer treatment are based on the use of molecules which contain a large number of  ${}^{10}\text{B}$ -atoms, e.g., the  $\text{Na}_3[\text{B}_{10}\text{H}_{12}\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2]$  molecule, other similar molecules, and molecular clusters [21], [22] (see also [23] and references therein). In this case the overall energy release from the reaction, Eq.(31), in one cancer cell can be extremely large. Correspondingly, the local temperature in the whole cell suddenly increases to very large values and this kills the incident cancer cell with almost 100 % probability. Note that the tritium nucleus does not form in the nuclear reaction Eq.(31) which means that it is safe to initiate this reaction inside of a human body. By studying the nuclear reaction, Eq.(1), in few-electron atoms and ions we want to develop a number of reliable theoretical methods and numerical procedures which can be later used in applications to the analogous reaction,

Eq.(31).

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TABLE I: An example of the trial, three-electron wave function constructed with the use of  $N = 23$  semi-exponential radial basis functions, Eq.(7). This wave function produces the total energy  $E = -7.44859276608$  *a.u.* for the ground  $^2S$ -state of the  $^\infty\text{Li}$  atom. Only one electron spin-function  $\chi_1 = \alpha\beta\alpha - \beta\alpha\alpha$  was used in these calculations.

$k$	$m_1(k)$	$m_2(k)$	$m_3(k)$	$C_k$	$\alpha_k$	$\beta_k$	$\gamma_k$
1	0	0	1	0.146131429481911E+02	0.416423958308045E+01	0.390330393520923E+01	0.754647967615054E+00
2	1	0	1	0.110681883475133E+03	0.526120133598745E+01	0.699723209902291E+01	0.604874234309236E+00
3	1	1	1	0.234004890152000E+03	0.598950989816454E+01	0.378246213278597E+01	0.590931685390717E+00
4	2	0	1	0.116882861303726E+03	0.413820964104499E+01	0.322650638788059E+01	0.590283203974117E+00
5	0	0	0	-0.112533836667930E+02	0.404234943769060E+01	0.402575246908481E+01	0.136870242306376E+01
6	0	0	2	0.124148253762594E+01	0.772078877480103E+01	0.208089611437233E+01	0.906692873308709E+00
7	0	0	3	0.129950444032051E+01	0.125634586976915E+02	0.167180833975207E+02	0.111484879880926E+01
8	3	0	1	0.121940082563610E+02	0.336154087416427E+01	0.329089537444583E+01	0.569461303170668E+00
9	2	2	1	-0.815264312642982E+01	0.315618697991587E+01	0.293590042487235E+01	0.642752252837086E+00
10	0	0	4	0.231307852206996E-01	0.216119418842614E+01	0.354528921898964E+01	0.848100637437686E+00
11	1	0	0	-0.290323204459308E+02	0.303111504960694E+01	0.340407714984374E+01	0.439831339492880E+00
12	1	0	2	-0.782805087195444E+01	0.319874342329211E+01	0.294880236447181E+01	0.670201325893484E+00
13	4	0	1	0.466451849833029E+05	0.257191421047538E+02	0.198922117452300E+02	0.745721864825035E+00
14	5	0	1	0.102312737866967E+03	0.610735801244370E+01	0.126738573321754E+02	0.583192334409026E+00
15	1	1	0	0.496831723313492E+01	0.214720891197913E+01	0.139151014500059E+02	0.332004403600092E+00
16	1	1	2	0.331570408306929E+01	0.313893628304852E+01	0.288670468153774E+01	0.656255394173358E+00
17	2	0	0	-0.224488896165048E+03	0.111494404746535E+02	0.712253949382151E+01	0.412242317869619E+00
18	2	0	2	-0.200426722868461E+01	0.282336074847368E+01	0.292360100848728E+01	0.638644442755579E+00
19	0	0	5	0.186252350189224E-02	0.103900277658347E+02	0.241603283627644E+01	0.858660133717424E+00
20	2	1	1	0.314011900712871E+01	0.314575640023816E+01	0.238785024725699E+01	0.645792868876097E+00
21	3	0	2	0.164525876141841E+01	0.318702139403640E+01	0.348200049008609E+01	0.663487519449685E+00
22	3	0	0	0.549306690646211E+01	0.313423005590041E+01	0.376361954006700E+01	0.494738425712773E+00
23	3	1	1	0.489167893642778E+01	0.310583281642480E+01	0.299668864388672E+01	0.617551331047668E+00

TABLE II: The probabilities (in %) of observing selected electron final states in the helium ion  ${}^4\text{He}^+$  and tritium atom  ${}^3\text{H}$  arising in the exothermic nuclear reaction Eq.(1) of the three-electron lithium-6 atom in its ground  ${}^2S$ -state with slow neutrons.

atom/state	$1s$	$2s$	$2p$
${}^4\text{He}^+$	$9.52386 \cdot 10^{-2}$	$1.66605 \cdot 10^{-2}$	$6.60170 \cdot 10^{-4}$
${}^3\text{H}$	$2.49810 \cdot 10^{-3}$	$3.05880 \cdot 10^{-4}$	$2.00251 \cdot 10^{-6}$